Fluid description of a system of classical particles

Girish S Setlur

1 General Formalism

The number density and current density of a fluid (by implication we want to disregard the discreteness of the particles in this point of view) made of discrete particles may be defined as (where $\delta(\mathbf{r}) = \delta(x)\delta(y)\delta(z)$ is the 3D Dirac delta function and $\mathbf{r} = (x, y, z)$)

$$\rho(\mathbf{r}, t) \; = \; \sum_{i=1}^{N} \delta(\mathbf{r} - \mathbf{r}_i(t)) \tag{1}$$

and

$$\mathbf{J}(\mathbf{r}, t) \; = \; \sum_{i=1}^{N} \mathbf{v}_i(t) \; \delta(\mathbf{r} - \mathbf{r}_i(t)) \tag{2}$$

where

$$\mathbf{v}_i(t) \; = \; \frac{d}{dt}\mathbf{r}_i(t) \tag{3}$$

Now,

$$\frac{\partial}{\partial t}\rho(\mathbf{r}, t) \; = \; -\sum_{i=1}^{N} \frac{d\mathbf{r}_i(t)}{dt} \cdot \nabla_{\mathbf{r}}\delta(\mathbf{r} - \mathbf{r}_i(t)) \tag{4}$$

Also,

$$\nabla \cdot \mathbf{J}(\mathbf{r}, t) \; = \; \sum_{i=1}^{N} \mathbf{v}_i(t) \; \cdot \nabla_{\mathbf{r}}\delta(\mathbf{r} - \mathbf{r}_i(t)) \tag{5}$$

This means,

$$\frac{\partial}{\partial t}\rho(\mathbf{r}, t) + \nabla \cdot \mathbf{J}(\mathbf{r}, t) \; = \; 0 \tag{6}$$

The above is called the continuity equation and is always valid regardless of what forces are or are not acting on the particles. In other words the continuity equation is a kinematic statement just like $\mathbf{v}_i(t) = \frac{d}{dt}\mathbf{r}_i(t)$. But the time derivative of the current density will involve acceleration which depends on what forces are acting.

$$\frac{\partial}{\partial t}\mathbf{J}(\mathbf{r}, t) \; = \; \sum_{i=1}^{N} \frac{d\mathbf{v}_i(t)}{dt} \; \delta(\mathbf{r} - \mathbf{r}_i(t)) - \sum_{i=1}^{N} \mathbf{v}_i(t) \; (\mathbf{v}_i(t) \cdot \nabla_{\mathbf{r}})\delta(\mathbf{r} - \mathbf{r}_i(t)) \tag{7}$$

The goal now is to write down $\frac{\partial}{\partial t}\mathbf{J}(\mathbf{r}, t)$ in terms of $\rho, \mathbf{J}$ again, without involving $\mathbf{r}_i$ or $\mathbf{v}_i$. When this is done, this equation together with the continuity equation will provide the complete fluid description of the N-particle system only in terms of $\rho, \mathbf{J}$ with no reference to the individual particles that make up the system. To do this we make the following assumptions. Assume that the Dirac delta function has been made less singular (which can be made singular at the end by taking the limit $\epsilon \to 0$) as follows $\delta(\mathbf{r}) = \delta_\epsilon(x)\delta_\epsilon(y)\delta_\epsilon(z)$ where,

$$\delta_\epsilon(x) \ = \ \frac{\epsilon/\pi}{x^2+\epsilon^2} \tag{8}$$

In this case $\delta(0)$ makes mathematical sense. Note that we may write,

$$\rho(\mathbf{r}_j(t),t) \ = \ \delta(0) \tag{9}$$

and

$$\mathbf{J}(\mathbf{r}_j(t),t) \ = \ \mathbf{v}_j(t)\ \delta(0) \tag{10}$$

These two are valid if, as we shall assume, $\mathbf{r}_i(t) = \mathbf{r}_j(t)$ only if $i = j$. This means,

$$\mathbf{v}_j(t) = \frac{\mathbf{J}(\mathbf{r}_j(t),t)}{\rho(\mathbf{r}_j(t),t)} \tag{11}$$

Now the term below may be simplified as follows:

$$\sum_{i=1}^{N} \mathbf{v}_i(t)\ (\mathbf{v}_i(t)\cdot\nabla_{\mathbf{r}})\delta(\mathbf{r}-\mathbf{r}_i(t)) \ = \ \sum_{i=1}^{N} \frac{\mathbf{J}(\mathbf{r}_i(t),t)}{\rho(\mathbf{r}_i(t),t)}\ (\mathbf{v}_i(t)\cdot\nabla_{\mathbf{r}})\delta(\mathbf{r}-\mathbf{r}_i(t)) \tag{12}$$

Now $\delta_{\mathbf{r}}$ does not act on $\mathbf{r}_i$ so we may write ($\frac{d}{dx}fg = f'g + fg'$),

$$\sum_{i=1}^{N} \frac{\mathbf{J}(\mathbf{r}_i(t),t)}{\rho(\mathbf{r}_i(t),t)}\ (\mathbf{v}_i(t)\cdot\nabla_{\mathbf{r}})\delta(\mathbf{r}-\mathbf{r}_i(t)) = \sum_{i=1}^{N}(\mathbf{v}_i(t)\cdot\nabla_{\mathbf{r}})[\frac{\mathbf{J}(\mathbf{r}_i(t),t)}{\rho(\mathbf{r}_i(t),t)}\ \delta(\mathbf{r}-\mathbf{r}_i(t))] = \sum_{i=1}^{N}(\mathbf{v}_i(t)\cdot\nabla_{\mathbf{r}})[\delta(\mathbf{r}-\mathbf{r}_i(t))\frac{\mathbf{J}(\mathbf{r},t)}{\rho(\mathbf{r},t)}] \tag{13}$$

The last because $\delta(\mathbf{r}-\mathbf{a})f(\mathbf{r}) = \delta(\mathbf{r}-\mathbf{a})f(\mathbf{a})$. Now,

$$\sum_{i=1}^{N}(\mathbf{v}_i(t)\cdot\nabla_{\mathbf{r}})[\delta(\mathbf{r}-\mathbf{r}_i(t))\frac{\mathbf{J}(\mathbf{r},t)}{\rho(\mathbf{r},t)}] \ = \ \frac{\mathbf{J}(\mathbf{r},t)}{\rho(\mathbf{r},t)}\sum_{i=1}^{N}(\mathbf{v}_i(t)\cdot\nabla_{\mathbf{r}})[\delta(\mathbf{r}-\mathbf{r}_i(t))] + (\sum_{i=1}^{N}\mathbf{v}_i(t)\delta(\mathbf{r}-\mathbf{r}_i(t))\cdot\nabla_{\mathbf{r}})\frac{\mathbf{J}(\mathbf{r},t)}{\rho(\mathbf{r},t)} \tag{14}$$

But,

$$\sum_{i=1}^{N}(\mathbf{v}_i(t)\cdot\nabla_{\mathbf{r}})[\delta(\mathbf{r}-\mathbf{r}_i(t))] \ = \ \nabla_{\mathbf{r}}\cdot\sum_{i=1}^{N}\mathbf{v}_i(t)\ \delta(\mathbf{r}-\mathbf{r}_i(t)) \ = \ \nabla_{\mathbf{r}}\cdot\mathbf{J}(\mathbf{r},t) \tag{15}$$

This means,

$$\sum_{i=1}^{N} \mathbf{v}_i(t)\ (\mathbf{v}_i(t)\cdot\nabla_{\mathbf{r}})\delta(\mathbf{r}-\mathbf{r}_i(t)) \ = \ \frac{\mathbf{J}(\mathbf{r},t)}{\rho(\mathbf{r},t)}\nabla_{\mathbf{r}}\cdot\mathbf{J}(\mathbf{r},t) + (\mathbf{J}(\mathbf{r},t)\cdot\nabla_{\mathbf{r}})\frac{\mathbf{J}(\mathbf{r},t)}{\rho(\mathbf{r},t)} \tag{16}$$

At this stage it is easy to see the wisdom in defining the velocity field of a fluid (as opposed to individual particles) as,

$$\mathbf{v}(\mathbf{r},t) \ = \ \frac{\mathbf{J}(\mathbf{r},t)}{\rho(\mathbf{r},t)} \tag{17}$$

This means,

$$\sum_{i=1}^{N} \mathbf{v}_i(t)\ (\mathbf{v}_i(t)\cdot\nabla_{\mathbf{r}})\delta(\mathbf{r}-\mathbf{r}_i(t)) \ = \ \mathbf{v}(\mathbf{r},t)\nabla_{\mathbf{r}}\cdot(\rho(\mathbf{r},t)\mathbf{v}(\mathbf{r},t)) + \rho(\mathbf{r},t)(\mathbf{v}(\mathbf{r},t)\cdot\nabla_{\mathbf{r}})\mathbf{v}(\mathbf{r},t) \tag{18}$$

Similarly we have to make sense of the first term on the right hand side of Eq.(7). But for this we have to know what forces are acting on the particle since acceleration is involved. The forces are of two types, one is a force due to an external source such as forces felt by the particles due to external pressure on the fluid. Or it could also be due to the particles interacting with each other due to forces such as van der Waals interaction and other two-body interactions. We will assume all these forces are conservative and derivable from a potential energy. In this case we write the following expression for the potential energy of a particle labelled "i".

$$U(\mathbf{r}_i) \;=\; V_{ext}(\mathbf{r}_i) + \sum_{j \neq i} v(\mathbf{r}_i - \mathbf{r}_j) \tag{19}$$

where the second term is the influence of all other particles on this particle "i". The first term is due to an external force such as force exerted by the walls of the container (pressure). The net force $\mathbf{F}(\mathbf{r}) \;=\; -\nabla_{\mathbf{r}} U(\mathbf{r})$.

$$m\frac{d\mathbf{v}_i(t)}{dt} \;=\; \mathbf{F}(\mathbf{r}_i(t)) \;=\; \int d\mathbf{r}^{'} \;\delta(\mathbf{r}^{'} - \mathbf{r}_i(t))\; \mathbf{F}(\mathbf{r}^{'}) \tag{20}$$

or,

$$m\frac{d\mathbf{v}_i(t)}{dt} \;=\; -\int d\mathbf{r}^{'} \;\delta(\mathbf{r}^{'} - \mathbf{r}_i(t))\nabla_{\mathbf{r}^{'}}\; (V_{ext}(\mathbf{r}^{'}) + \sum_j v(\mathbf{r}^{'} - \mathbf{r}_j)) \tag{21}$$

(we assert that $v(0) = 0$ so that we avoid repeatedly writing $i \neq j$). This means the first term in Eq.(7)

$$\sum_{i=1}^{N} \frac{d\mathbf{v}_i(t)}{dt}\; \delta(\mathbf{r} - \mathbf{r}_i(t)) \;=\;$$

$$-\frac{1}{m}\int d\mathbf{r}^{'} \;\sum_{i=1}^{N} \delta(\mathbf{r} - \mathbf{r}_i(t))\; \delta(\mathbf{r}^{'} - \mathbf{r}_i(t))\nabla_{\mathbf{r}^{'}}\; V_{ext}(\mathbf{r}^{'}) - \frac{1}{m}\int d\mathbf{r}^{'} \;\sum_{i=1}^{N} \delta(\mathbf{r} - \mathbf{r}_i(t))\; \delta(\mathbf{r}^{'} - \mathbf{r}_i(t))\nabla_{\mathbf{r}^{'}}\; \sum_j v(\mathbf{r}^{'} - \mathbf{r}_j) \tag{22}$$

or,

$$\sum_{i=1}^{N} \frac{d\mathbf{v}_i(t)}{dt}\; \delta(\mathbf{r} - \mathbf{r}_i(t)) \;=\;$$

$$-\frac{1}{m}\int d\mathbf{r}^{'} \;\sum_{i=1}^{N} \delta(\mathbf{r} - \mathbf{r}^{'})\; \delta(\mathbf{r}^{'} - \mathbf{r}_i(t))\nabla_{\mathbf{r}^{'}}\; V_{ext}(\mathbf{r}^{'}) - \frac{1}{m}\int d\mathbf{r}^{'} \;\sum_{i=1}^{N} \delta(\mathbf{r} - \mathbf{r}^{'})\; \delta(\mathbf{r}^{'} - \mathbf{r}_i(t))\nabla_{\mathbf{r}^{'}}\; \sum_j v(\mathbf{r}^{'} - \mathbf{r}_j) \tag{23}$$

or,

$$\sum_{i=1}^{N} \frac{d\mathbf{v}_i(t)}{dt}\; \delta(\mathbf{r} - \mathbf{r}_i(t)) \;=\; -\frac{1}{m}\int d\mathbf{r}^{'} \;\delta(\mathbf{r} - \mathbf{r}^{'})\; \rho(\mathbf{r}^{'},t)\nabla_{\mathbf{r}^{'}}\; V_{ext}(\mathbf{r}^{'}) - \frac{1}{m}\int d\mathbf{r}^{'} \;\delta(\mathbf{r} - \mathbf{r}^{'})\; \rho(\mathbf{r}^{'},t)\nabla_{\mathbf{r}^{'}}\; \sum_j v(\mathbf{r}^{'} - \mathbf{r}_j) \tag{24}$$

or,

$$\sum_{i=1}^{N} \frac{d\mathbf{v}_i(t)}{dt}\; \delta(\mathbf{r} - \mathbf{r}_i(t)) \;=\; -\frac{1}{m}\rho(\mathbf{r},t)\nabla_{\mathbf{r}}\; V_{ext}(\mathbf{r}) - \frac{1}{m}\;\rho(\mathbf{r},t)\nabla_{\mathbf{r}}\; \sum_j v(\mathbf{r} - \mathbf{r}_j) \tag{25}$$

Similarly,

$$\sum_j v(\mathbf{r} - \mathbf{r}_j) \;=\; \sum_j \int d\mathbf{r}^{'}\; v(\mathbf{r} - \mathbf{r}^{'})\; \delta(\mathbf{r}^{'} - \mathbf{r}_j) \;=\; \int d\mathbf{r}^{'}\; v(\mathbf{r} - \mathbf{r}^{'})\; \sum_j \delta(\mathbf{r}^{'} - \mathbf{r}_j) \;=\; \int d\mathbf{r}^{'}\; v(\mathbf{r} - \mathbf{r}^{'})\; \rho(\mathbf{r}^{'}) \tag{26}$$

Thus,

$$\sum_{i=1}^{N} \frac{d\mathbf{v}_i(t)}{dt}\ \delta(\mathbf{r}-\mathbf{r}_i(t)) \ = \ -\frac{1}{m}\rho(\mathbf{r},t)\nabla_{\mathbf{r}}\ V_{ext}(\mathbf{r}) - \frac{1}{m}\ \rho(\mathbf{r},t)\nabla_{\mathbf{r}}\ \int d\mathbf{r}^{'}\ v(\mathbf{r}-\mathbf{r}^{'})\ \rho(\mathbf{r}^{'},t) \tag{27}$$

All this allows us to write Eq.(7) only in terms of ρ and $\mathbf{J}$ (or equivalently, ρ and $\mathbf{v}$) instead of involving $\mathbf{r}_i, \mathbf{v}_i$.

$$\frac{\partial}{\partial t}\mathbf{J}(\mathbf{r},t) \ = \ -\frac{1}{m}\rho(\mathbf{r},t)\nabla_{\mathbf{r}}\ V_{ext}(\mathbf{r}) - \frac{1}{m}\ \rho(\mathbf{r},t)\nabla_{\mathbf{r}}\ \int d\mathbf{r}^{'}\ v(\mathbf{r}-\mathbf{r}^{'})\ \rho(\mathbf{r}^{'},t) - \mathbf{v}(\mathbf{r},t)\nabla_{\mathbf{r}}\cdot(\rho(\mathbf{r},t)\mathbf{v}(\mathbf{r},t)) - \rho(\mathbf{r},t)(\mathbf{v}(\mathbf{r},t)\cdot\nabla_{\mathbf{r}})\mathbf{v}(\mathbf{r},t) \tag{28}$$

when there are no mutual interactions between particle i.e. when $v(\mathbf{r}) \equiv 0$ the above equation is called the Euler equation. When mutual interactions are present, it is called Boltzmann equation.

2 The Boltzmann Equation

The continuity equation (equation for $\frac{\partial}{\partial t}\rho$) together with the Euler-Boltzmann equation (equation for $\frac{\partial}{\partial t}\mathbf{J}$ or $\frac{\partial}{\partial t}\rho\mathbf{v}$) form a replacement for the huge (Avagadro) number of equations that we may write down using Newton's Laws:
(i.e. $\frac{d^2}{dt^2}\mathbf{r}_i(t) = \frac{1}{m}\mathbf{F}(\mathbf{r}_i(t))$; $i = 1, 2, 3, ..., N = 10^{23}$). For this we first we define the convective derivative as

$$\frac{D}{Dt} \ \equiv \ \frac{\partial}{\partial t} + \mathbf{v}(\mathbf{r},t)\cdot\nabla_{\mathbf{r}} \tag{29}$$

This means the continuity equation (Eq.(6)) may be written as,

$$\frac{D}{Dt}\ \rho(\mathbf{r},t) + \rho(\mathbf{r},t)\nabla\cdot\mathbf{v}(\mathbf{r},t) \ = \ 0 \tag{30}$$

and the Boltzmann equation is (I have skipped many steps **ASSIGNMENT:** Derive Eq.(30) and Eq.(31) using equations of earlier section: Due date: 14 Oct 2021),

$$m\frac{D}{Dt}\mathbf{v}(\mathbf{r},t) \ = \ -\nabla_{\mathbf{r}}\ V_{eff}(\mathbf{r},t) \tag{31}$$

where,

$$V_{eff}(\mathbf{r},t) \ = \ V_{ext}(\mathbf{r}) + \int d\mathbf{r}^{'}\ v(\mathbf{r}-\mathbf{r}^{'})\ \rho(\mathbf{r}^{'},t) \tag{32}$$

It is remarkable that the Boltzmann equation Eq.(31) resembles Newton's Law (mass times acceleration equals force), although here we are talking about the entire fluid and the acceleration includes convective terms.